ECE 371
Materials and Devices
HW #1
Due: 09/03/19 at the beginning of class

*All problems from Neamen 4th Edition Ch. 1

1.1 Determine the number of atoms per unit cell in a (*a*) face-centered cubic, (*b*) body-centered cubic, and (*c*) diamond lattice.

1.2 Assume that each atom is a hard sphere with the surface of each atom in contact with the surface of its nearest neighbor. Determine the percentage of total unit cell volume that is occupied in (*a*) a simple cubic lattice, (*b*) a face-centered cubic lattice, (*c*) a body-centered cubic lattice, and (*d*) a diamond lattice.

1.3 If the lattice constant of silicon is 5.43 Å, calculate (*a*) the distance from the center of one silicon atom to the center of its nearest neighbor, (*b*) the number density of silicon atoms (#/cm^3), and (*c*) the mass density (g/cm^3) of silicon.

1.7 Assume the radius of an atom, which can be represented as a hard sphere, is $r = 1.95$ Å. The atom is placed in a (*a*) simple cubic, (*b*) fcc, (*c*) bcc, and (*d*) diamond lattice. Assuming that nearest atoms are touching each other, what is the lattice constant of each lattice?

1.8 A crystal is composed of two elements, A and B. The basic crystal structure is a face-centered cubic with element A at each of the corners and element B in the center of each face. The effective radius of element A is $r_A = 1.035$ Å. Assume that the elements are hard spheres with the surface of each A-type atom in contact with the surface of its nearest A-type neighbor. Calculate (*a*) the maximum radius of the B-type element that will fit into this structure, (*b*) the lattice constant, and (*c*) the volume density (#/cm^3) of both the A-type atoms and the B-type atoms.

1.11 The crystal structure of sodium chloride (NaCl) is a simple cubic with the Na and Cl atoms alternating positions. Each Na atom is then surrounded by six Cl atoms and likewise each Cl atom is surrounded by six Na atoms. (*a*) Sketch the atoms in a (100) plane. (*b*) Assume the atoms are hard spheres with nearest neighbors touching. The effective radius of Na is 1.0 Å and the effective radius of Cl is 1.8 Å. Determine the lattice constant. (*c*) Calculate the volume density of Na and Cl atoms. (*d*) Calculate the mass density of NaCl.

1.15 The lattice constant of a simple cubic lattice is a_0. (*a*) Sketch the following planes: (i) (110), (ii) (111), (iii) (220), and (iv) (321). (*b*) Sketch the following directions: (i) [110], (ii) [111], (iii) [220], and (iv) [321].

1.16 For a simple cubic lattice, determine the Miller indices for the planes shown in Figure P1.16.

1.18 The lattice constant of a simple cubic primitive cell is 5.28 Å. Determine the distance between the nearest parallel (*a*) (100), (*b*) (110), and (*c*) (111) planes.

1.19 The lattice constant of a single crystal is 4.73 Å. Calculate the surface density (#/cm^2) of atoms on the (i) (100), (ii) (110), and (iii) (111) plane for a (*a*) simple cubic, (*b*) body-centered cubic, and (*c*) face-centered cubic lattice.

1.25 (*a*) Assume that 2×10^{16} cm^{-3} of boron atoms are distributed homogeneously throughout single crystal silicon. What is the fraction by weight of boron in the crystal? (*b*) If phosphorus atoms, at a concentration of 10^{18} cm^{-3}, are added to the material in part (*a*), determine the fraction by weight of phosphorus.

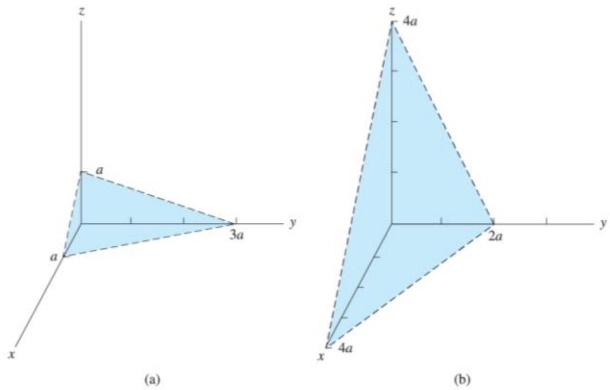


Figure P1.16 | Figure for Problem 1.16.

1.1 Determine the number of atoms per unit cell in a (*a*) face-centered cubic, (*b*) body-centered cubic, and (*c*) diamond lattice.

(a) FCC — 6 faces $\times \frac{1}{2}$ atom = 3 atoms

8 corners $\times \frac{1}{8}$ atom = 1 atom

$$\boxed{4 \ \frac{\text{atoms}}{\text{unit}}}$$

(b) BCC — 1 center = 1 atom

8 corners $\times \frac{1}{8}$ atom = 1 atom

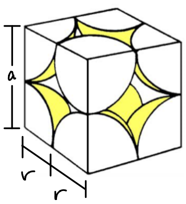
$$\boxed{2 \ \frac{\text{atoms}}{\text{unit}}}$$

(c) Diamond — 2 FCC

$$\boxed{8 \ \frac{\text{atoms}}{\text{unit}}}$$

1.2 Assume that each atom is a hard sphere with the surface of each atom in contact with the surface of its nearest neighbor. Determine the percentage of total unit cell volume that is occupied in (*a*) a simple cubic lattice, (*b*) a face-centered cubic lattice, (*c*) a body-centered cubic lattice, and (*d*) a diamond lattice.

(a) SC

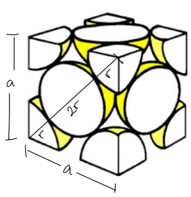


$$\text{unit vol.} = 1\,\frac{\text{atom}}{\text{unit}} \times \frac{4}{3}\pi r^3 = \frac{4}{3}\pi r^3$$

$$\text{cubic vol} = a^3 \rightarrow a = 2r \longrightarrow 8r^3$$

$$\frac{\text{unit}}{\text{cubic}} = \frac{\frac{4}{3}\pi \cancel{r^3}}{8\cancel{r^3}} = \frac{4}{24}\pi \approx \boxed{52.36\%}$$

(b) FCC



$$\text{unit vol.} = 4\,\frac{\text{atom}}{\text{unit}} \times \frac{4}{3}\pi r^3 = \frac{16}{3}\pi r^3$$

$$\text{cubic vol.} = a^3 \qquad (4r)^2 = a^2 + a^2$$

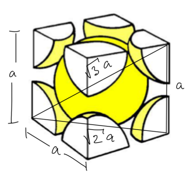
$$= (2\sqrt{2}r)^3 \qquad \cancel{16}r^2 = \cancel{2}a^2$$

$$= (8(2^{3/2})r^3) \qquad 8r^2 = a^2$$

$$a = 2\sqrt{2}\,r$$

$$\frac{\text{unit}}{\text{cubic}} = \frac{\cancel{16}\pi \cancel{r^3}}{3\cdot\cancel{16}\sqrt{2}\,\cancel{r^3}} \approx \boxed{74.05\%}$$

(c) BCC



$$\text{unit vol.} = 2\,\frac{\text{atom}}{\text{unit}} \times \frac{4}{3}\pi r^3 = \frac{8}{3}\pi r^3$$

$$\text{cube vol.} = a^3 \rightarrow (4r)^2 = a^2 + (\sqrt{2}a)^2$$

$$16r^2 = 3a^2$$

$$a = \frac{\sqrt{16r^2}}{\sqrt{3}} = \frac{4r}{\sqrt{3}}$$

$$\frac{\text{unit}}{\text{cubic}} = \frac{\frac{8}{3}\pi \cancel{r^3}}{\frac{64\cancel{r^3}}{3^{3/2}}} \approx \boxed{68.02\%}$$

(d) Diamond

$$\text{unit vol.} = 8 \frac{\text{atom}}{\text{unit}} \times \frac{4}{3}\pi r^3 = \frac{32\pi r^3}{3}$$

$$\text{diamond vol.} = a^3 \qquad (8r)^2 = a^2 + (\sqrt{2}a)^2$$

$$= \left(\frac{8r}{\sqrt{3}}\right)^3 \qquad 64r^2 = 3a^2$$

$$a = \frac{\sqrt{64r^2}}{\sqrt{3}} = \frac{8r}{\sqrt{3}}$$

$$\frac{\text{unit}}{\text{diamond}} = \frac{\frac{32\pi \cancel{r^3}}{3}}{\left(\frac{8\cancel{r}}{\sqrt{3}}\right)^3} \approx \boxed{34.01\%}$$

1.3 If the lattice constant of silicon is 5.43 Å, calculate (*a*) the distance from the center of one silicon atom to the center of its nearest neighbor, (*b*) the number density of silicon atoms ($\#/cm^3$), and (*c*) the mass density (g/cm^3) of silicon.

$a = 5.43 \times 10^{-8}\,cm$

silicon → diamond lattice

(a) $a = \frac{8r}{\sqrt{3}} \rightarrow r = \frac{\sqrt{3}}{8} a$

$= 1.1756 \times 10^{-8}\,cm$

$\text{center-to-center} = 2r = \boxed{2.3513 \times 10^{-8}\,cm}$

(b) $\frac{\#\,\text{atoms}}{cm^3} = \frac{8}{a^3} = \frac{8}{1.6010 \times 10^{-22}} = \boxed{4.9968 \times 10^{-22} \frac{\text{atoms}}{cm^3}}$

(c) $\frac{\text{grams}}{cm^3} = \frac{\left(\frac{\#\,\text{atoms}}{cm^3}\right)\left(\text{atomic mass}\right)}{\text{Avogadro's }\#}$

$= \frac{(4.996 \times 10^{-22})(28.085)}{6.022 \times 10^{23}} = \boxed{2.3304 \frac{\text{grams}}{cm^3}}$

1.7 Assume the radius of an atom, which can be represented as a hard sphere, is $r = 1.95$ Å. The atom is placed in a (*a*) simple cubic, (*b*) fcc, (*c*) bcc, and (*d*) diamond lattice. Assuming that nearest atoms are touching each other, what is the lattice constant of each lattice?

$r = 1.95 \times 10^{-8}$ cm

(a) SC — $a = 2r = \boxed{3.9 \times 10^{-8} \text{ cm}}$

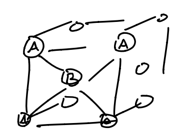
(b) FCC — $a = 2\sqrt{2}\,r = \boxed{5.5154 \times 10^{-8} \text{ cm}}$

(c) BCC — $a = \frac{4r}{\sqrt{3}} = \boxed{4.5033 \times 10^{-8} \text{ cm}}$

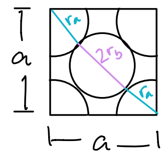
(d) Diamond — $a = \frac{8r}{\sqrt{3}} = \boxed{9.067 \times 10^{-8} \text{ cm}}$

1.8 A crystal is composed of two elements, A and B. The basic crystal structure is a face-centered cubic with element A at each of the corners and element B in the center of each face. The effective radius of element A is $r_A = 1.035$ Å. Assume that the elements are hard spheres with the surface of each A-type atom in contact with the surface of its nearest A-type neighbor. Calculate (*a*) the maximum radius of the B-type element that will fit into this structure, (*b*) the lattice constant, and (*c*) the volume density (#/cm^3) of both the A-type atoms and the B-type atoms.

FCC



$r_a = 1.035$



(a) $a = 2r = 2(1.035\times10^{-8}) = 2.07\times10^{-8}\,\text{cm}$

$$a^2 + a^2 = (r_a + 2r_b + r_a)^2$$

$$\sqrt{a^2+a^2} = r_a + 2r_b + r_a$$

$$\sqrt{2}\,a = 2r_a + 2r_b$$

$$\frac{\sqrt{2}\,a - 2r_a}{2} = r_b \rightarrow \frac{(\sqrt{2})(2.07\times10^{-8}) - 2(1.035)}{2}$$

$$\boxed{r_b = 4.2817\times10^{-9}\,\text{cm}}$$

(b) from part (a): $\boxed{a = 2.07\times10^{-8}\,\text{cm}}$

(c) FCC $\rightarrow$ 4 atoms $\rightarrow$ 3 face (B)
1 corner (A)

$$B - \frac{\#\,\text{atoms}}{\text{cm}^3} = \frac{3}{(2.07\times10^{-8})^3} = \boxed{3.3823\times10^{23}}$$

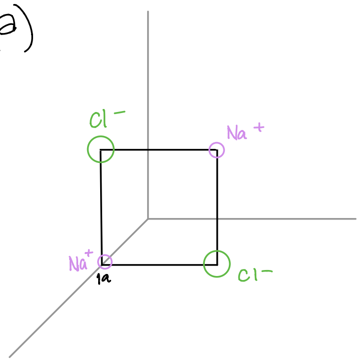
$$A - \frac{\#\,\text{atoms}}{\text{cm}^3} = \frac{1}{(2.07\times10^{-8})^3} = \boxed{1.1274\times10^{23}}$$

1.11 The crystal structure of sodium chloride (NaCl) is a simple cubic with the Na and Cl atoms alternating positions. Each Na atom is then surrounded by six Cl atoms and likewise each Cl atom is surrounded by six Na atoms. (*a*) Sketch the atoms in a (100) plane. (*b*) Assume the atoms are hard spheres with nearest neighbors touching. The effective radius of Na is 1.0 Å and the effective radius of Cl is 1.8 Å. Determine the lattice constant. (*c*) Calculate the volume density of Na and Cl atoms. (*d*) Calculate the mass density of NaCl.

$r_{Na} = 1.0 \times 10^{-8}$ cm

$r_{Cl} = 1.8 \times 10^{-8}$ cm

(a)



(b) $$\boxed{\begin{aligned} a &= r_{Na} + r_{Cl} \\ &= 2.8 \times 10^{-8} \text{ cm} \end{aligned}}$$

(c) $$\text{Na}- \frac{\#\text{ atoms}}{\text{cubic}} = \frac{\frac{1}{2}}{(2.8\times10^{-8})^3} = \boxed{2.2777\times10^{22} \frac{\text{atoms}}{\text{cm}^3}}$$

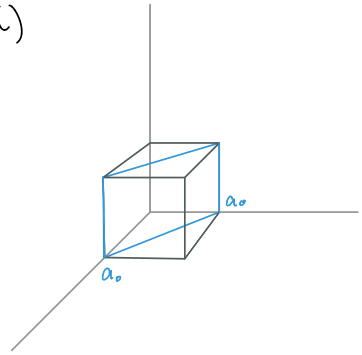
$$\text{Cl}- \frac{\#\text{atoms}}{\text{cubic}} = \frac{\frac{1}{2}}{(2.8\times10^{-8})^3} = \boxed{2.2777\times10^{22} \frac{\text{atoms}}{\text{cm}^3}}$$

(d) $$\frac{(\#\text{atoms})(\text{atomic mass})}{\text{avogadro's }\#} = \frac{(\frac{1}{2})(22.9897)+(\frac{1}{2})(35.45)}{6.022\times10^{23}}$$

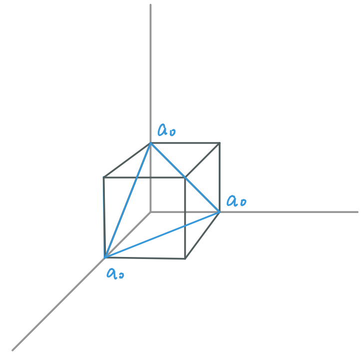
$$\boxed{= 4.8522\times10^{-23} \frac{\text{grams}}{\text{cubic}}}$$

1.15 The lattice constant of a simple cubic lattice is a_0. (*a*) Sketch the following planes: (i) (110), (ii) (111), (iii) (220), and (iv) (321). (*b*) Sketch the following directions: (i) [110], (ii) [111], (iii) [220], and (iv) [321].

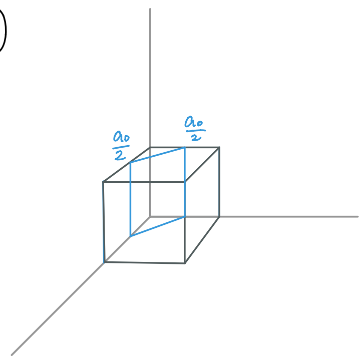
(a) (i)

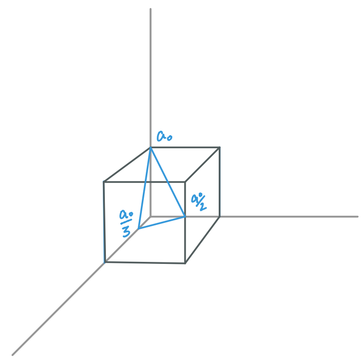


(ii)

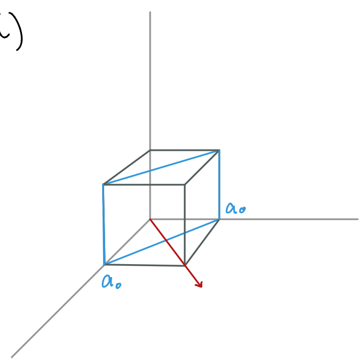


(iii)

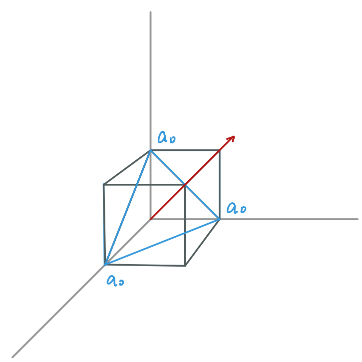




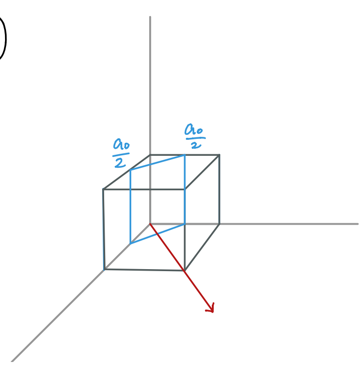
(b) (i)

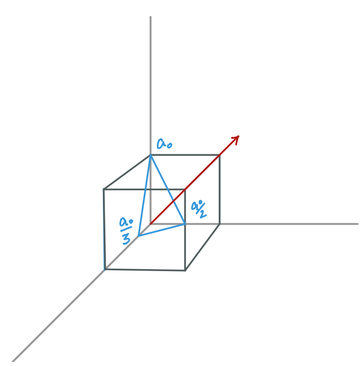


(ii)



(iii)





1.16 For a simple cubic lattice, determine the Miller indices for the planes shown in Figure P1.16.

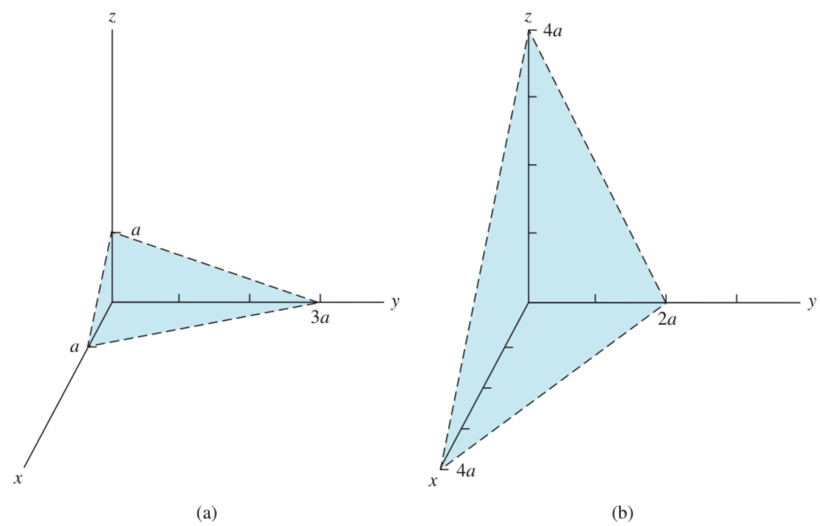


Figure P1.16 | Figure for Problem 1.16.

(a) 1 3 1 $\rightarrow$ $\frac{1}{1}\ \frac{1}{3}\ \frac{1}{1}$ $\rightarrow$ $\boxed{(3\ 1\ 3)}$

(b) 4 2 4 $\rightarrow$ $\frac{1}{4}\ \frac{1}{2}\ \frac{1}{4}$ $\rightarrow$ $\boxed{(1\ 2\ 1)}$

1.18 The lattice constant of a simple cubic primitive cell is 5.28 Å. Determine the distance between the nearest parallel (*a*) (100), (*b*) (110), and (*c*) (111) planes.

(a) $d = a = 5.28 \times 10^{-8}$ cm

(b) $d = \frac{a}{\sqrt{2}} = 3.7335 \times 10^{-8}$ cm

(c) $d = \frac{a}{\sqrt{3}} = 3.0484 \times 10^{-8}$ cm

1.19 The lattice constant of a single crystal is 4.73 Å. Calculate the surface density (#/cm²) of atoms on the (i) (100), (ii) (110), and (iii) (111) plane for a (*a*) simple cubic, (*b*) body-centered cubic, and (*c*) face-centered cubic lattice.

(a) (i) $(100) \rightarrow \dfrac{1}{(4.73\times10^{-8})^2} = 4.4697\times10^{14}$

(ii) $(110) \rightarrow \dfrac{1}{(4.73\times10^{-8})^2\sqrt{2}} = 3.1606\times10^{14}$

(iii) $(111) \rightarrow \dfrac{1}{(4.73\times10^{-8})^2\sqrt{3}} = 2.5806\times10^{14}$

(b) (i) $(100) \rightarrow \dfrac{1}{(4.73\times10^{-8})^2} = 4.4697\times10^{14}$

(ii) $(110) \rightarrow \dfrac{2}{(4.73\times10^{-8})^2\sqrt{2}} = 6.3211\times10^{14}$

(iii) $(111) \rightarrow \dfrac{1}{(4.73\times10^{-8})^2\sqrt{3}} = 2.5806\times10^{14}$

(c) (i) $(100) \rightarrow \dfrac{2}{(4.73\times10^{-8})^2} = 8.9394\times10^{14}$

(ii) $(110) \rightarrow \dfrac{2}{(4.73\times10^{-8})^2\sqrt{2}} = 6.3211\times10^{14}$

(iii) $(111) \rightarrow \dfrac{4}{(4.73\times10^{-8})^2\sqrt{3}} = 1.0322\times10^{15}$

1.25 (*a*) Assume that 2×10^{16} cm^{-3} of boron atoms are distributed homogeneously throughout single crystal silicon. What is the fraction by weight of boron in the crystal? (*b*) If phosphorus atoms, at a concentration of 10^{18} cm^{-3}, are added to the material in part (*a*), determine the fraction by weight of phosphorus.

(a) Fraction by weight $= \dfrac{(2\times10^{16})(10.82)}{(5\times10^{22})(28.085)} = \boxed{1.5410\times10^{-7}}$

(b) Fraction by weight $= \dfrac{(10^{18})(30.9738)}{(2\times10^{16})(10.82)+(5\times10^{22})(28.085)}$

$$\boxed{= 2.2057\times10^{-5}}$$